# Higher order Schmidt decompositions

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**Abstract**

Necessary and sufficient conditions are given for the existence of extended Schmidt decompositions, with more than two subspaces.

Schmidt's theorem [1, 2] has a fundamental importance in the quantum theory of measurement. In the simple case of finite dimensional spaces [3, 4], the theorem asserts that any double sum

$$\Psi = \sum_{mn} A_{mn}\, x_m\, y_n\,, \tag{1}$$

can be converted into a single sum

$$\Psi = \sum_{\mu} a_\mu\, \xi_\mu\, \eta_\mu\,, \tag{2}$$

by means of *unitary* transformations

$$\xi_\mu = \sum_m U_{\mu m}\, x_m \qquad \text{and} \qquad \eta_\mu = \sum_n V_{\mu n}\, y_n\,. \tag{3}$$

If $\{x_m\}$ and $\{y_n\}$ are two orthonormal bases for two distinct vector spaces, then $\{\xi_\mu\}$ and $\{\eta_\mu\}$ also are two, possibly incomplete, orthonormal vector bases for these two spaces.

The absolute values $|a_\mu|$ are called the *singular values* [3] of the matrix $A$, and are easily calculated by noting that $|a_\mu|^2$ are the nonvanishing eigenvalues of the Hermitian matrices $AA^\dagger$ and $A^\dagger A$. The corresponding sets of eigenvectors are $\{\xi_\mu\}$ and $\{\eta_\mu\}$, respectively.

A natural question is whether this process can be extended to more than two subspaces. Such an extension of Schmidt's theorem would be useful for modal interpretations of quantum theory, and triple sums can indeed sometimes be found in the literature on that subject [5–7]. Although none of these last references is technically wrong, because of the context where these triple sums appear, they may give the impression that multiple Schmidt decompositions are always possible. I have actually seen such a false assumption used in a preprint, already accepted for publication, whose author will be eternally grateful to me for warning him of the error before it was too late.

The unlikeliness of occurence of multiple Schmidt decompositions can readily be seen by counting the free parameters involved: for example, if there are three particles, each of which described by a $d$-dimensional space, their combined (pure) state, in a $d^3$-dimensional space, depends on $2(d^3-1)$ real parameters (after discarding overall normalization and phase factors). On the other hand, the three unimodular unitary transformations which can be performed for these three particles have only $3(d^2-1)$ free parameters, not enough to solve the problem in general.

This negative result prompts a more difficult question: what are the necessary and sufficient conditions for the occurence of a triple, or multiple, Schmidt decomposition? Consider a triple sum

$$\Psi = \sum_{mns} A_{mns}\, x_m\, y_n\, z_s\,, \tag{4}$$

where $\{x_m\}$, $\{y_n\}$ and $\{z_s\}$ are three orthonormal bases in three distinct vector spaces. Can we rewrite the above expression as $\sum a_\mu \xi_\mu \eta_\mu \zeta_\mu$, with three orthonormal sets, $\{\xi_\mu\}$, $\{\eta_\mu\}$ and $\{\zeta_\mu\}$? Schmidt's theorem only asserts that Eq. (4) can be unitarily converted into

$$\Psi = \sum_\mu a_\mu\, \xi_\mu\, \omega_\mu\,, \tag{5}$$

where $\{\xi_\mu\}$ is a set of orthonormal vectors in the space that was spanned by $\{x_m\}$, and $\{\omega_\mu\}$ is a set of orthonormal vectors in the space spanned by the set $\{y_n \otimes z_s\}$.

Consider first, for simplicity, the case where all the $|a_\mu|$ are different, so that the decomposition (5) is unique. We can then write, if a triple Schmidt decomposition exists,

$$\forall\mu \qquad \omega_\mu = \sum_{ns} \mathit{\Omega}_{\mu ns}\, y_n\, z_s = \eta_\mu\, \zeta_\mu\,. \tag{6}$$

This implies that all the $\Omega_\mu$ matrices, namely the matrices with elements $(\Omega_\mu)_{ns} = \Omega_{\mu ns}$, are of rank 1, and satisfy both $\Omega_\mu^\dagger\,\Omega_\nu = 0$ and $\Omega_\mu\,\Omega_\nu^\dagger = 0$ if $\mu \neq \nu$. These conditions are obviously necessary. They are also sufficient, because if they hold, we can obtain orthogonal sets $\{\eta_\mu\}$ and $\{\zeta_\mu\}$ as the eigenvectors of $\Omega_\mu^\dagger\,\Omega_\mu$ and $\Omega_\mu\,\Omega_\mu^\dagger$, respectively.

If several nonvanishing $|a_\mu|$ are equal, the decomposition (5) is not unique, and the situation becomes more complicated. Suppose that $n$ of these $|a_\mu|$ are equal, so that the corresponding $\xi_\mu$ and $\omega_\mu$ are defined only up to an arbitrary unitary transformation, represented by a matrix of order $n$. Consider the subspace spanned by these $\omega_\mu$. Then, obviously, the corresponding $\Omega_\mu$ matrices should be of a rank not exceeding $n$. Moreover, there should be $n$ linear combinations of the $\Omega_\mu$ matrices, generated by the inverse of the above unitary transformation, such that the resulting matrices, $\Omega'_\mu$ say, are all of rank 1, and satisfy orthogonality conditions as specified above for the nondegenerate case, namely $\Omega'^\dagger_\mu\,\Omega'_\nu = 0$ and $\Omega'_\mu\,\Omega'^\dagger_\nu = 0$ if $\mu \neq \nu$. This completes the solution of this problem.

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1. E. Schmidt, Math. Ann. 63 (1907) 433.

2. F. Riesz and B. Sz.-Nagy, Functional analysis (Ungar, New York, 1955) p. 243.

3. P. Lancaster and M. Tismenetsky, The theory of matrices (Academic Press, Boston, 1985) p. 182.

4. A. Peres, Quantum theory: concepts and methods (Kluwer, Dordrecht, 1993) p. 123.

5. S. Kochen, in "Symposium on the foundations of modern physics" ed. by P. Lahti and P. Mittelstaedt (World Scientific, Singapore, 1985) p. 151.

6. E. J. Squires, in "Quantum theory without reduction" ed. by M. Cini and J.-M. Lévy-Leblond (Hilger, Bristol, 1990) p. 151.

7. R. Healey, Found. Phys. Letters 6 (1993) 37.

8. L. E. Ballentine, Am. J. Phys. 63 (1995) 285.